On Polynomial Preconditioning and Asymptotic Convergence Factors for Indefinite Hermitian Matrices*

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ABSTRACT

We are concerned with the minimal residual method combined with polynomial preconditioning for solving large linear systems $Ax = b$ with indefinite Hermitian coefficient matrices A. The standard approach for choosing the polynomial preconditioner leads to preconditioned systems which are positive definite. Here, we investigate a different strategy which leaves the preconditioned coefficient matrix indefinite. More precisely, the polynomial preconditioner is designed to cluster the positive (negative) eigenvalues of A around 1 (around some negative constant). In particular, it is shown that such indefinite polynomial preconditioners can be obtained as the optimal solutions of a certain two-parameter family of Chebyshev approximation problems. The problem of selecting the parameters so that the resulting indefinite polynomial preconditioner speeds up the convergence of the minimal residual method optimally is also addressed. For this task, we propose an approach based on the concept of asymptotic convergence factors. Finally, some numerical examples of indefinite polynomial preconditioners are given.

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1. INTRODUCTION

Conjugate gradient type algorithms combined with preconditioning are among the most effective iterative procedures for solving large sparse nonsingular linear systems

$$Ax = b. \tag{1.1}$$

In recent years, polynomial preconditioning has attracted much interest. The technique consists of selecting a polynomial s of small degree and then applying a conjugate gradient type method to one of the two linear systems

$$s(A)Ax = s(A)b \tag{1.2}$$

(left preconditioning) or

$$As(A)y = b, \qquad x = s(A)y \tag{1.3}$$

(right preconditioning). Notice that, as long as $s(A)$ is nonsingular, (1.2) and (1.3) are both equivalent to the original linear system (1.1). Moreover, the systems (1.2) and (1.3) have the same coefficient matrix $s(A)A = As(A)$. Clearly, the polynomial s should be chosen such that the conjugate gradient iteration for (1.2) or (1.3) converges as fast as possible.

For the case of Hermitian positive definite A, the idea goes back to Rutishauser [23], who proposed polynomial preconditioning in the fifties as a remedy for roundoff in the classical conjugate gradient (CG) algorithm of Hestenes and Stiefel [16]. The recent revival [17] of Rutishauser's method and the general interest in polynomial preconditioning is mainly motivated by the attractive features of this technique for vector and parallel computers (see [24] for a survey).

In this note, we are concerned with polynomial preconditioning for linear systems (1.1) with Hermitian, but indefinite coefficient matrices A. An obvious strategy for the design of the preconditioner is to choose s such that $s(A)A$ is as close as possible to the identity matrix I. This approach was studied in detail by Ashby [2] and Ashby, Manteuffel, and Saylor [3]. We remark that the resulting preconditioned system (1.2) or (1.3) is then Hermitian positive definite and thus can be solved by the standard CG algorithm.

In this paper, we study a second preconditioning strategy which, in contrast to the first approach, leaves the preconditioned matrix $s(A)A$ indefinite. Roughly speaking, s is chosen such that $s(A)A$ is as close as

possible to I on the positive part of the spectrum of A and as close as possible to μI, where $\mu \in \mathbb{R}$ is some negative constant, on the negative part of the spectrum of A. In particular, we will show how polynomials s of this type can be obtained as solutions of a family of Chebyshev approximation problems depending on two parameters, namely μ and a weight factor $w \in \mathbb{R}$. The problem of selecting the parameters such that the resulting indefinite polynomial preconditioner speeds up the convergence of the minimal residual method optimally is also addressed. For this task, we propose an approach based on the concept of asymptotic convergence factors. Finally, note that, since the resulting matrix $s(A)A$ is now indefinite, the standard CG algorithm is no longer suitable for solving (1.2) or (1.3), and we use the minimal residual (MR) method instead.

The paper is organized as follows. In Section 2, we recall a few basic properties of the MR method. In Section 3, we derive an explicit formula for the asymptotic convergence factor of the MR iteration based on the knowledge of two intervals which contain all eigenvalues of A. Also, a numerical procedure for computing asymptotic convergence factors is outlined. In Section 4, a two-parameter family of Chebyshev approximation problems is introduced, and some basic properties are listed. In Section 5, we consider indefinite polynomial preconditioners and show that there is an intimate connection with the class of approximation problems investigated in the previous section. Some numerical examples of indefinite polynomial preconditioners and their associated asymptotic convergence factors are presented in Section 6. Finally, we make some concluding remarks in Section 7.

Throughout this paper, A is assumed to be a nonsingular Hermitian, but indefinite $N \times N$ matrix. $\sigma(A)$ denotes the spectrum of A, and $\|x\|_2 = \sqrt{x^H x}$ is the Euclidean norm of $x \in \mathbb{C}^N$. Moreover, the notation Π_n will be used for the set of all complex polynomials of degree at most n. Finally, we denote by $\Pi_n^{(r)}$ the subclass which consists of all real polynomials in Π_n.

2. THE MINIMAL RESIDUAL METHOD. ERROR BOUNDS

Let $x_0 \in \mathbb{C}^N$ be any initial guess for the exact solution $A^{-1}b$ of (1.1), and let $r_0 := b - Ax_0$ be the corresponding residual vector. Moreover, we denote by

$$K_n := \operatorname{span}\{r_0, Ar_0, A^2 r_0, \ldots, A^{n-1} r_0\} \tag{2.1}$$

the nth Krylov subspace of $\mathbb{C}^N$ generated by r_0 and A. Starting from x_0, the

MR method generates a sequence of approximations x_n, $n = 1, 2, \ldots$, to $A^{-1}b$ which are uniquely defined by the minimal residual property

$$\|b - Ax_n\|_2 = \min_{x \in x_0 + K_n} \|b - Ax\|_2, \qquad x_n \in x_0 + K_n. \tag{2.2}$$

The MR method was first introduced by Stiefel [25] as a variant of the classical CG method for Hermitian positive definite matrices A. However, the algorithm given in [25] may break down (see e.g. [5,9]) if A is indefinite. A numerically stable implementation—based on the Lanczos algorithm [19] —of the MR approach for indefinite Hermitian matrices was first devised by Paige and Saunders [21].

As is typical for CG-type methods, in exact arithmetic, the MR method is a finite procedure. More precisely (see e.g. [5,9]), $x_m = A^{-1}b$, where m is given as the minimal number of components in any expansion of r_0 into orthonormal eigenvectors of A, i.e.

$$r_0 = \sum_{j=1}^{m} \rho_j u_j, \tag{2.3}$$

where $\rho_j > 0$, $Au_j = \lambda^{(j)} u_j$, $\lambda^{(1)} < \lambda^{(2)} < \cdots < \lambda^{(m)}$, and

$$u_j^H u_k = \begin{cases} 1 & \text{if} \quad j = k, \\ 0 & \text{if} \quad j \neq k. \end{cases}$$

However, in practice, the iterative character of CG methods is usually more important than the finite termination property. In particular, for the choice of a suitable preconditioner for a CG-type algorithm, it is crucial to have error bounds for its iterates. Next, we state such estimates for the MR method.

For this purpose, some information on the location of the eigenvalues of A is necessary. Here and in the sequel, we assume that two intervals $[a, b]$ and $[c, d]$ are known such that

$$\sigma(A) \subset [a, b] \cup [c, d], \qquad \text{where} \quad c < d < 0 < a < b. \tag{2.4}$$

Note that, ideally, b (c) would be the largest (smallest) eigenvalue of A, and a (d) the smallest positive (largest negative) eigenvalue.

By the standard technique, expressing the Krylov subspace (2.1) $K_n = \{q(A)r_0 | q \in \Pi_{n-1}\}$ in terms of polynomials and using the expansion (2.3) of r_0, one readily deduces from (2.2) the following result.

THEOREM 2.1. *For* $n = 1, 2, \ldots,$

$$\frac{\|b - Ax_n\|_2}{\|b - Ax_0\|_2} \leq E_n(a, b, c, d), \tag{2.5}$$

where $E_n(a, b, c, d)$ *is the optimal value of the approximation problem*

$$(E_n(a, b, c, d) :=) \min_{p \in \Pi_n^{(r)}: p(0) = 1} \max_{\lambda \in [a, b] \cup [c, d]} |p(\lambda)|. \tag{2.6}$$

Note that the outlined derivation of the bound (2.5) actually leads to the complex version of (2.6) with Π_n instead of $\Pi_n^{(r)}$. Standard results (e.g. [20]) from approximation theory guarantee that there always exists a unique optimal polynomial p_n^* for this complex approximation problem. Moreover, it is easily verified (cf. [20, Theorem 27]) that p_n^* is real, and therefore it is sufficient to consider only polynomials $p \in \Pi_n^{(r)}$ in (2.6).

Unfortunately, the solution of (2.6) is explicitly known only for special cases. For example, it is well known (see e.g. [2]) that for intervals of equal length $b - a = d - c$ the optimal polynomials are suitably transformed Chebyshev polynomials. The solution of (2.6) is also known for a variety of other parameters a, b, c, d, and can be found in the classical work of Achieser [1] (see also Peherstorfer [22, Section 5]). For the general case, there is no closed expression for the optimal value $E_n(a, b, c, d)$ of (2.6). However, it is known that for $n \to \infty$ this quantity behaves like κ^n, where $\kappa = \kappa(a, b, c, d) \in (0, 1)$. More precisely,

$$\lim_{n \to \infty} [E_n(a, b, c, d)]^{1/n} =: \kappa(a, b, c, d) \quad \text{and} \quad 0 < \kappa(a, b, c, d) < 1 \tag{2.7}$$

(see Eiermann, Niethammer, and Varga [8], where this result is established for more general sets in the complex plane). $\kappa(a, b, c, d)$ is called the *asymptotic convergence factor*.

3. COMPUTATION OF THE ASYMPTOTIC CONVERGENCE FACTOR FOR TWO INTERVALS

In this section, we are concerned with the actual computation of the asymptotic convergence factor $\kappa(a, b, c, d)$ (2.7).

As Eiermann, Li, and Varga [7] pointed out, asymptotic convergence factors—not only for the union of two real intervals, but for more general compact sets $\Omega \subset \mathbb{C}$—can be expressed in terms of the Green's function $G(\lambda;\infty)$ (see e.g. [26, pp. 65]) for $\Omega^c := \hat{\mathbb{C}} \setminus \Omega$ with pole at infinity. Note that the existence of $G(\lambda;\infty)$ is guaranteed if Ω^c is of finite connectivity; moreover, the Green's function is then uniquely defined by the following three properties:

(i) $G(\cdot;\infty)$ is a real harmonic function on $\mathbb{C} \setminus \Omega$.

(ii) There is a $\lambda_* \in \mathbb{R}$ such that $G(\lambda;\infty) - \log|\lambda|$ is harmonic for all $\lambda \in \hat{\mathbb{C}}$ with $|\lambda| \geq \lambda_*$.

(iii) $\lim_{\lambda \to \lambda_0} G(\lambda;\infty) = 0$ for all $\lambda_0 \in \partial\Omega$.

For $\Omega = [a,b] \cup [c,d]$, the set Ω^c is doubly connected, and by applying the results from [7, Section 3] it follows that

$$\kappa(a,b,c,d) = \exp[-G(0;\infty)]. \tag{3.1}$$

Next, we use the connection (3.1) with the Green's function to derive a representation of $\kappa(a,b,c,d)$ in terms of elliptic integrals.

First, let $\Omega^c \subset \hat{\mathbb{C}}$ be any doubly connected region with $\infty \in \Omega^c$. Suppose we know a conformal mapping

$$f: A_r \to \Omega^c, \qquad \text{with} \quad f(A_r) = \Omega^c, \tag{3.2}$$

of some annulus

$$A_r := \{z \in \mathbb{C} \mid r < |z| < 1\}, \qquad \text{with} \quad 0 < r < 1, \tag{3.3}$$

onto Ω^c. Moreover, it is assumed that

$$\tau := f^{-1}(\infty) \quad \text{satisfies} \quad r < \tau < 1. \tag{3.4}$$

Note that (3.4) can always be achieved by a simple rotation in the z-plane. By means of f, the problem of finding the Green's function for Ω^c can be reduced to that of determining the Green's function $G_r(z;\tau)$ for the annulus A_r with pole at τ. More precisely, the identity

$$G(\lambda;\infty) = G_r(f^{-1}(\lambda);\tau), \qquad \lambda \in \Omega^c, \tag{3.5}$$

holds (e.g. [15, p. 259]). However, there are explicit representations for

$G_r(z;\tau)$. Here we will use the following formula (see [15, pp. 259]):

$$G_r(z;\tau) = \left(\frac{\log|z|}{\log r} - 1\right)\log\tau - \log\left|\frac{\sum_{j=-\infty}^{\infty} r^{j^2}[-z/(r\tau)]^j}{\sum_{j=-\infty}^{\infty} r^{j^2}[-\tau z/r]^j}\right|. \quad (3.6)$$

From now on, let $\Omega := [a,b]\cup[c,d]$. So far, we have shown that, by means of (3.1), (3.5), and (3.6), the desired quantity $\kappa(a,b,c,d)$ can be expressed in terms of $f^{-1}(0)$, where f is a conformal mapping satisfying (3.2)–(3.4). Such functions f are explicitly known (see e.g. Kober's dictionary of conformal representations [18, pp. 191]) and are of the form

$$f(z) = f_{k,\tau}(z) := \frac{a-b}{2}\frac{\mathrm{sn}^2\left(\frac{K'}{\pi}\log z;k\right) + \mathrm{sn}^2\left(\frac{K'}{\pi}\log\tau;k\right)}{\mathrm{sn}^2\left(\frac{K'}{\pi}\log z;k\right) - \mathrm{sn}^2\left(\frac{K'}{\pi}\log\tau;k\right)} + \frac{a+b}{2}. \quad (3.7)$$

Here, $w = \mathrm{sn}(u;k)$ is the Jacobian elliptic function (see e.g. [13, pp. 904]) defined—via its inverse $u = \mathrm{sn}^{-1}(w;k)$—by

$$u = \mathrm{sn}^{-1}(w;k) = \int_0^w \frac{d\xi}{\sqrt{(1-\xi^2)(1-k^2\xi^2)}}. \quad (3.8)$$

The real number k is a parameter (the *modulus* of sn) with $k \in [0,1]$. The number K' in (3.7) is not a free parameter, but depends on k:

$$K' = K'(k) := \int_0^{\pi/2} \frac{d\varphi}{\sqrt{1-(1-k^2)\sin^2\varphi}} \left[= \mathrm{sn}^{-1}\left(1;\sqrt{1-k^2}\right)\right]. \quad (3.9)$$

Similarly, we set

$$K = K(k) := \int_0^{\pi/2} \frac{d\varphi}{\sqrt{1-k^2\sin^2\varphi}} \left[= \mathrm{sn}^{-1}(1;k)\right]. \quad (3.10)$$

Note that $\mathrm{sn}(u;k)$ is a doubly periodic meromorphic function with periods

$4K$ and $2iK'$ and poles at the points $2mK+(2n+1)iK'$, $m,n \in \mathbb{Z}$. Finally, we remark that the branch of the logarithm in (3.7) is chosen such that

$$\log z = \log|z| + i \arg z, \qquad -\pi < \arg z \leqslant \pi.$$

Using standard techniques from complex analysis, it is readily verified that the function (3.7) indeed maps an annulus A_r of the type (3.3) conformally onto the complement of two disjoint real intervals. Here, the inner radius r of A_r is given by

$$r = r(k) := \exp\left(\frac{-\pi K(k)}{K'(k)}\right). \tag{3.11}$$

Moreover, the image of the outer boundary $|z| = 1$ of A_r under f is just the interval $[a,b]$. Hence, it only remains to adjust the two free parameters k and τ in (3.7) so that the inner boundary $|z| = r$ of A_r is mapped onto $[c,d]$. This requirement leads to the two equations

$$\frac{a-b}{2}\,\frac{1+\mathrm{sn}^2(M;k)}{1-\mathrm{sn}^2(M;k)} + \frac{a+b}{2} = c, \tag{3.12a}$$

$$\frac{a-b}{2}\,\frac{1/k^2+\mathrm{sn}^2(M;k)}{1/k^2-\mathrm{sn}^2(M;k)} + \frac{a+b}{2} = d, \tag{3.12b}$$

where we have set

$$M = M(k,\tau) := \frac{K'(k)\log\tau}{\pi}. \tag{3.13}$$

By solving first (3.12a) for $\mathrm{sn}^2(M;k)$ and subsequently (3.12b) for k^2, we obtain

$$\mathrm{sn}(M;k) = -\sqrt{\frac{a-c}{b-c}} \quad \text{and} \quad k = \sqrt{\frac{(a-d)(b-c)}{(a-c)(b-d)}}. \tag{3.14}$$

Note that, by (3.4) and (3.13), $M < 0$, and thus, in view of (3.8), also

$\mathrm{sn}(M;k) < 0$. By (3.14) and (3.13), the two free parameters k and τ in (3.7) and the function f are now uniquely determined. By (3.1) and (3.5), we have

$$\kappa(a,b,c,d) = \exp[-G_r(z_0;\tau)], \qquad \text{where} \quad z_0 := f^{-1}(0). \tag{3.15}$$

Therefore, it remains to determine the solution z_0 of $f(z) = 0$. To this end, we set

$$u_0 = \frac{K'}{\pi} \log z_0 \quad \text{or, equivalently,} \quad z_0 = \exp\left(\frac{\pi u_0}{K'}\right). \tag{3.16}$$

Using (3.7) and the first relation in (3.14), it follows that u_0 is the solution of

$$\mathrm{sn}(u_0;k) = \sqrt{\frac{b}{a}}\ \mathrm{sn}(M;k) = -\sqrt{\frac{b(a-c)}{a(b-c)}}\ . \tag{3.17}$$

Next, recall (e.g. [13, p. 914]) the identity

$$\mathrm{sn}(v + iK';k) \equiv \frac{1}{k\ \mathrm{sn}(v;k)}\ . \tag{3.18}$$

By means of (3.18), (3.16), and (3.14), we deduce from (3.17) that

$$u_0 = v_0 + iK', \qquad v_0 := -\mathrm{sn}^{-1}\left(\sqrt{\frac{a(b-d)}{b(a-d)}}\ ;k\right), \quad \text{and} \quad z_0 = -\exp\left(\frac{\pi v_0}{K'}\right). \tag{3.19}$$

Finally, using (3.15), (3.6) (with $z = z_0$), (3.11), (3.13), and (3.19), one arrives at the formula

$$\kappa(a,b,c,d) = \exp\left[\left(1 + \frac{v_0}{K}\right)\frac{\pi M}{K'}\right] \times \frac{\sum_{j=-\infty}^{\infty} \exp\left(-\pi \frac{K}{K'} j^2 + \frac{\pi}{K'}(v_0 - M + K)j\right)}{\sum_{j=-\infty}^{\infty} \exp\left(-\pi \frac{K}{K'} j^2 + \frac{\pi}{K'}(v_0 + M + K)j\right)}. \tag{3.20}$$

For the numerical evaluation of (3.20) it is advantageous to rewrite (3.20). To this end, let

$$\theta(z,\lambda) := \sum_{j=-\infty}^{\infty} \exp(-\pi\lambda j^2 + 2izj) \tag{3.21}$$

be one of the theta functions (see e.g. [13, p. 921]). By means of (3.21), it follows from (3.20) that

$$\kappa(a,b,c,d) = \exp\left[\left(1+\frac{v_0}{K}\right)\frac{\pi M}{K'}\right]\frac{\theta(z_1,\lambda_0)}{\theta(z_2,\lambda_0)}, \tag{3.22}$$

where

$$\lambda_0 = \frac{K}{K'}, \qquad z_1 = \frac{\pi}{2iK'}(v_0 - M + K), \qquad z_2 = \frac{\pi}{2iK'}(v_0 + M + K).$$

A straightforward computation, using Jacobi's identity (see e.g. [14, p. 272])

$$\theta(z,\lambda) \equiv \frac{1}{\sqrt{\lambda}}\exp\left(\frac{-z^2}{\pi\lambda}\right)\theta\left(\frac{z}{i\lambda},\frac{1}{\lambda}\right)$$

with $\lambda = \lambda_0$ and $z = z_1$ respectively $z = z_2$, shows that the representation (3.22) is equivalent to the final formula (3.24) stated in the following theorem. Furthermore, by the variable transformation $\xi = w/\sqrt{t+1}$ in (3.8), we have expressed the elliptic integrals which occur in (3.9), (3.10), (3.14), and (3.19) in terms of the standard form

$$R_F(x,y,z) := \frac{1}{2}\int_0^{\infty} \frac{dt}{\sqrt{(t+x)(t+y)(t+z)}}, \qquad x,y,z \geqslant 0, \tag{3.23}$$

of the elliptic integral of the first kind.

THEOREM 3.1. *Let $c < d < 0 < a < b$. Then*

$$\kappa(a,b,c,d) = \frac{\vartheta_4\left(\pi\dfrac{v_0 - M}{2K}, q\right)}{\vartheta_4\left(\pi\dfrac{v_0 + M}{2K}, q\right)}, \tag{3.24}$$

$$\vartheta_4(\psi, q) := 1 + 2\sum_{j=1}^{\infty} (-1)^j q^{j^2} \cos(2\psi j),$$

where

$$q = \exp\left(\frac{-\pi K'}{K}\right), \qquad k = \sqrt{\frac{(a-d)(b-c)}{(a-c)(b-d)}}, \qquad K = R_F(1,0,1-k^2),$$

$$K' = R_F(1,0,k^2), \qquad M = -\sqrt{\frac{a-c}{b-c}}\, R_F\left(1, \frac{b-a}{b-c}, \frac{b-a}{b-d}\right), \tag{3.25}$$

$$v_0 = -\sqrt{\frac{a(b-d)}{b(a-d)}}\, R_F\left(1, \frac{d(a-b)}{b(a-d)}, \frac{c(a-b)}{b(a-c)}\right).$$

Next, using the representation (3.24) and (3.25) of the asymptotic convergence factor κ, we deduce the following

COROLLARY 3.2.

(a) *$\kappa(a,b,c,d)$ is a continuous function on $\{(a,b,c,d) \in \mathbb{R}^4 | c < d < 0 < a < b\}$.*

(b) *Let $\{a_n\}_{n\in\mathbb{N}}$, $\{b_n\}_{n\in\mathbb{N}}$, $\{c_n\}_{n\in\mathbb{N}}$, and $\{d_n\}_{n\in\mathbb{N}}$ be given convergent sequences with limits a, b, c, and d, respectively. Moreover, assume that $c_n < d_n < 0 < a_n < b_n$ for all $n \in \mathbb{N}$ and that $c < d \leqslant 0 \leqslant a < b$. If $a = 0$ and/or $d = 0$, then*

$$\lim_{n\to\infty} \kappa(a_n, b_n, c_n, d_n) = 1.$$

Proof. First, note that all the operations in (3.24) and (3.25) are continuous as long as $c < d < 0 < a < b$ holds, and part (a) is obviously true. We now turn to the proof of part (b). Let $\kappa_n, q^{(n)}, k^{(n)}, \ldots, v_0^{(n)}$ denote the

quantities in (3.24) and (3.25) evaluated at a_n, b_n, c_n, d_n. We need to check their behavior for $n \to \infty$. There are three cases, namely

(i) $d = 0 < a$,
(ii) $d < 0 = a$,
(iii) $d = 0 = a$.

In cases (i) and (ii), the sequences $q^{(n)}, k^{(n)}, K^{(n)}, \ldots, v_0^{(n)}$ converge for $n \to \infty$ to finite limits $q, k, K, \ldots, v_0$, respectively, and $K > 0$. Furthermore, $v_0 = -K$ in case (i) and $v_0 = 0$ in case (ii). Therefore, in view of (3.24), κ_n converges to 1. Finally, consider case (iii). Here k_n converges to $k = 0$. By (3.10), (3.9), and (3.25), it follows that

$$\lim_{n \to \infty} K_n = 0, \qquad \lim_{n \to \infty} K_n' = \infty, \quad \text{and} \quad \lim_{n \to \infty} q_n = 0.$$

Using the definition of the theta function in (3.24), we deduce

$$\lim_{n \to \infty} \vartheta_4(\psi_n, q_n) = 1 \qquad \text{for all} \quad \psi_n \in \mathbb{R},$$

and hence, by (3.24), $\lim_{n \to \infty} \kappa_n = 1$. This concludes the proof of the corollary. ■

REMARK 3.3. The theta functions ϑ_4 and θ in (3.24) and (3.21), respectively, are connected through

$$\vartheta_4(\psi, q) \equiv \theta\left(\psi + \frac{\pi}{2}, -\frac{\log q}{\pi}\right), \qquad \psi \in \mathbb{R}, \quad 0 < q < 1.$$

There are whole books filled with the numerous properties and identities which hold for theta functions. In the sequel, we will make use of the relations

$$\vartheta_4(\pi/2, q) = \sqrt{2K/\pi} \tag{3.26}$$

and

$$\vartheta_4(\psi, q) = \prod_{j=1}^{\infty} (1 - 2q^{2j-1}\cos(2\psi) + q^{2(2j-1)})(1 - q^{2j})$$

$$\geqslant \vartheta_4(0, q) = \left(\frac{2K}{\pi}\sqrt{1-k^2}\right)^{1/2} \qquad \text{for all} \quad \psi \in \mathbb{R} \tag{3.27}$$

(see e.g. [13, pp. 921]). Here, q is defined in (3.25) with $K = K(k)$ and $K' = K'(k)$ given by (3.10) and (3.9).

By means of Theorem 3.1, the asymptotic convergence factor $\kappa(a, b, c, d)$ can be very easily computed numerically. For the calculation of the integrals R_F of the type (3.23), which occur in (3.25), there are standard algorithms. For the numerical examples presented in Section 6, we have used a procedure due to Carlson [4, Algorithm 1]. Finally, in (3.24), an infinite series needs to be computed twice. In the following, let $\psi \in \mathbb{R}$ and $J \in \mathbb{N}$. Moreover, suppressing the parameter q and the index 4, we set

$$\vartheta(\psi) := \vartheta_4(\psi, q) \quad \text{and} \quad \vartheta^{(J)}(\psi) := 1 + 2\sum_{j=1}^{J} (-1)^j q^{j^2} \cos(2\psi j). \tag{3.28}$$

If J is chosen large enough, the finite series $\vartheta^{(J)}(\psi)$ will yield a sufficiently accurate approximation to $\vartheta(\psi)$. We now derive a formula for such an integer J. Using (3.24), (3.28), (3.26), and the fact that $0 < q < 1$, one obtains

$$\begin{aligned} \left|\vartheta(\psi) - \vartheta^{(J)}(\psi)\right| &= 2\left|\sum_{j=J+1}^{\infty} (-1)^j q^{j^2} \cos(2\psi j)\right| \\ &\leqslant 2\sum_{j=J+1}^{\infty} q^{j^2} = 2q^{(J+1)^2} \sum_{j=0}^{\infty} q^{j^2+2j(J+1)} \leqslant 2q^{(J+1)^2} \sum_{j=0}^{\infty} q^{j^2} \\ &= q^{(J+1)^2}\left(1 + \vartheta_4(\pi/2, q)\right) = q^{(J+1)^2}\left(1 + \sqrt{2K/\pi}\right). \end{aligned} \tag{3.29}$$

With (3.28), (3.27), and (3.29), we arrive at the estimate

$$\left|\frac{\vartheta(\psi) - \vartheta^{(J)}(\psi)}{\vartheta(\psi)}\right| \leqslant q^{(J+1)} \frac{1 + [\pi/(2K)]^{1/2}}{(1-k^2)^{1/4}}. \tag{3.30}$$

From (3.30), it follows that the truncated series $\vartheta^{(J)}(\psi)$ approximates $\vartheta(\psi)$ with a relative error

$$\left|\frac{\vartheta(\psi) - \vartheta^{(J)}(\psi)}{\vartheta(\psi)}\right| \leqslant \epsilon,$$

if J is chosen as

$$J := [t], \qquad \text{where} \quad t := \left| \frac{\log\left[\epsilon(1-k^2)^{1/4}\right] + \log\left[1+[\pi/(2K)]^{1/2}\right]}{\log q} \right|^{1/2}.$$

Here, as usual, $[t]$ denotes the integer part of $t \in \mathbb{R}$.

We conclude this section by stating the following proposition, which is a special case of a more general result due to Eiermann, Li, and Varga [7, Proposition 3]. This monotonicity property of the asymptotic convergence factor κ will be used in Section 5.

PROPOSITION 3.4. *Let* $c \leqslant c' < d' \leqslant d < 0 < a \leqslant a' < b' \leqslant b$ *be given, and assume that at least one of the inequalities* "$\leqslant$" *is strict. Then*

$$\kappa(a', b', c', d') < \kappa(a, b, c, d).$$

4. A FAMILY OF CHEBYSHEV APPROXIMATION PROBLEMS

As we will see in the next section, the task of finding an optimal polynomial preconditioner for $Ax = b$ leads to a family of Chebyshev approximation problems. In this section, some results for such approximation problems are presented.

In the following, it is assumed that $S := [a, b] \cup [c, d]$ is the union of a positive and a negative interval with arbitrary, but fixed endpoints $c < d < 0 < a < b$. Moreover, $l \in \mathbb{N}$ always denotes a positive integer. Finally, set $\Gamma := \{(\mu, w) \in \mathbb{R} \times \mathbb{R} \mid w > 0\}$.

We will study the following family of approximation problems depending on the two parameters $(\mu, w) \in \Gamma$:

$$\gamma_l(\mu, w) := \min_{s \in \Pi_{l-1}^{(r)}} \|f - \lambda s\|_\omega, \qquad \|f - \lambda s\|_\omega := \max_{\lambda \in S} \left| \omega(\lambda)\left[f(\lambda) - \lambda s(\lambda)\right] \right|, \tag{4.1}$$

where

$$f(\lambda) = \begin{cases} 1 & \text{if} \quad \lambda > 0, \\ \mu & \text{if} \quad \lambda < 0, \end{cases} \qquad \omega(\lambda) = \begin{cases} 1 & \text{if} \quad \lambda > 0, \\ w & \text{if} \quad \lambda < 0. \end{cases} \tag{4.2}$$

REMARK 4.1. For the special case $\mu = w = 1$, (4.1) reduces to the approximation problem (2.6) (with n replaced by l) which arose in Section 2 in connection with error bounds for the MR method.

(4.1) is a linear Chebyshev approximation problem: we seek to approximate $f(\lambda)$ by polynomials of the form $\lambda s(\lambda) \in \Pi_l^{(r)}$ in the weighted uniform norm $\|\cdot\|_\omega$. Note that $0 \notin S$, and this guarantees that Haar's condition is satisfied. Standard results (see e.g. [20]) from approximation theory show that there always exists a unique optimal polynomial for (4.1) which is characterized by an equioscillation property. We summarize these results for (4.1) in the following

PROPOSITION 4.2. *Let $l \in \mathbb{N}$ and $(\mu, w) \in \Gamma$. Then:*

(a) *There exists a unique optimal polynomial $s_l^*(\lambda; \mu, w) \in \Pi_{l-1}^{(r)}$ for* (4.1).

(b) *$s \in \Pi_{l-1}^{(r)}$ is the optimal polynomial for* (4.1) *if, and only if, there exist $l+1$ extremal points*

$$c \leqslant \lambda_0 < \lambda_1 < \cdots < \lambda_{k_{\text{neg}}-1} \leqslant d, \qquad a \leqslant \lambda_{k_{\text{neg}}} < \lambda_{k_{\text{neg}}+1} < \cdots < \lambda_l \leqslant b \tag{4.3}$$

of $\omega(\lambda) - \lambda s(\lambda)$ and a number $y \in \mathbb{R}$ such that

$$\omega\big(\lambda_j\big[f(\lambda_j) - \lambda_j s(\lambda_j)\big]\big) = \begin{cases} (-1)^j y & \text{for } j = 0, 1, \ldots, k_{\text{neg}} - 1, \\ (-1)^{j-1} y & \text{for } j = k_{\text{neg}}, k_{\text{neg}} + 1, \ldots, l. \end{cases} \tag{4.4}$$

Moreover, if s is optimal, then $\gamma_l(\mu, w) = |y|$.

Here, a point $\lambda^* \in S$ is called an *extremal point* of $f - \lambda s(\lambda)$ if

$$\big|w(\lambda^*)\big[f(\lambda^*) - \lambda^* s(\lambda^*)\big]\big| = \|f - \lambda s\|_\omega.$$

The following corollary is a simple consequence of part (b) of Proposition 4.2.

COROLLARY 4.3. *Let $s_l^*(\lambda;\mu,w)$ be the optimal polynomial of* (4.1).

(a) $s_l^* \equiv 0$ *if, and only if,* $l=1$ *and* $w=1/\mu$.

(b) *Unless* $s_l^* \not\equiv 0$, *there are at least* $l+1$ *and at most* $l+3$ *extremal points of* $f-\lambda s_l^*$ *in* S. *Moreover, at most* $l-1$ *of these extremal points are contained in the interior* $(a,b)\cup(c,d)$ *of* S.

Proof. By using (4.3) and (4.4), one readily verifies part (a).

We now turn to part (b). First, note that, by part (b) of Proposition 4.2, $f-\lambda s_l^*$ has at least $l+1$ extremal points in S. Next, recall [cf. (4.2)] that f is constant for $\lambda>0$ and $\lambda<0$, respectively. Hence

$$\big[f(\lambda)-\lambda s_l^*(\lambda;\mu,w)\big]' = -\big[\lambda s_l^*(\lambda;\mu,w)\big]' =: p(\lambda) \qquad \text{for all} \quad \lambda\neq 0. \tag{4.5}$$

Now assume that $s_l^* \not\equiv 0$. Then p is a polynomial of degree not exceeding $l-1$, and $p\not\equiv 0$. This shows that p has at most $l-1$ zeros. On the other hand, in view of (4.5), $p(\lambda_j)=0$ for all extremal points $\lambda_j \in S\setminus\{a,b,c,d\}$ of $f-\lambda s_l^*$, and thus there are at most $l-1$ such "inner" extremal points λ_j. Therefore, altogether, there cannot be more than $l-1+4=l+3$ extremal points in S. ∎

In the next section, we will also make use of the fact that the optimal value of (4.1) depends continuously on the parameters μ and w.

LEMMA 4.4. *Let* $l\in\mathbb{N}$. *Then the optimal value* $\gamma_l(\mu,w)$ *of* (4.1) *is a continuous function of* $(\mu,w)\in\Gamma$.

We remark that, for w fixed, it follows from a standard result (see e.g. [27, Lemma 13.1]) in Chebyshev approximation theory that $\gamma_l(\mu,w)$ is a continuous function of μ. The proof given in [27] is easily adapted to the family of approximation problems (4.1).

Proof of Lemma 4.4. Let $\mu_1,\mu_2\in\mathbb{R}$, $w_1,w_2>0$ be arbitrary, and denote by $f_1,f_2,\omega_1,\omega_2$ the associated functions (4.2). Furthermore, assume that $l\in\mathbb{N}$ is fixed, and let s_1^* and s_2^* be the optimal polynomials of (4.1)

corresponding to (μ_1, w_1) and (μ_2, w_2), respectively. By using the optimality of s_1^*, the triangle inequality, and the obvious fact that $\|\cdot\|_{\omega_1} \leqslant \max\{1, w_1/w_2\}\|\cdot\|_{\omega_2}$, we obtain the estimates

$$\begin{aligned}\gamma_l(\mu_1, w_1) &= \|f_1 - \lambda s_1^*\|_{\omega_1} \leqslant \|f_1 - \lambda s_2^*\|_{\omega_1} \\ &\leqslant \|f_1 - f_2\|_{\omega_1} + \|f_2 - \lambda s_2^*\|_{\omega_1} \\ &\leqslant w_1|\mu_1 - \mu_2| + \max\{1, w_1/w_2\}\,\gamma_l(\mu_2, w_2). \qquad (4.6)\end{aligned}$$

With $\gamma_l(\mu_2, w_2) \leqslant \|f_2\|_{\omega_2} = \max\{1, |\mu_2|w_2\}$, it follows from (4.6) that

$$\gamma_l(\mu_1, w_1) - \gamma_l(\mu_2, w_2) \leqslant w_1|\mu_1 - \mu_2| + \max\left\{0, \frac{w_1 - w_2}{w_2}\right\}\max\{1, |\mu_2|w_2\}. \qquad (4.7)$$

Obviously, we may exchange the parameters (μ_1, w_1) and (μ_2, w_2) in (4.7). Therefore, (4.7) leads to the inequality

$$\begin{aligned}&|\gamma_l(\mu_1, w_1) - \gamma_l(\mu_2, w_2)| \\ &\leqslant |\mu_1 - \mu_2|\max\{w_1, w_2\} + |w_1 - w_2|\max\left\{\frac{1}{w_1}, \frac{1}{w_2}\right\}\max\{1, |\mu_1|w_1, |\mu_2|w_2\},\end{aligned}$$

which implies the continuity of $\gamma_l(\mu, w)$. ∎

REMARK 4.5. In general, $\gamma_l(\mu, w)$ is not differentiable. Typically, differentiability gets lost when the number $k_{\text{neg}} = k_{\text{neg}}(\mu, w)$ of negative extremal points in (4.3) and (4.4) changes. The following example illustrates this behavior. Let $l = 2$, $S = [1, 3] \cup [-2, -1]$, and $\mu = -2$ be fixed. It is straightforward to verify, by means of part (b) of Proposition 4.2, that the best polynomial $s^*(\lambda; w)$ and corresponding optimal value $\gamma(w)$ of (4.1) are given by

$$s^*(\lambda; w) = \frac{2(4 - \lambda)}{7}, \quad \gamma(w) = \frac{1}{7} \qquad \text{if} \quad 0 < w \leqslant 0.1,$$

and by

$$s^*(\lambda; w) = \frac{2(2-\lambda/\xi)}{\xi+2-1/\xi}, \quad \gamma(w) = \frac{\xi-2+1/\xi}{\xi+2-1/\xi},$$

$$\text{with} \quad \xi = 1+2\sqrt{\frac{3w}{1+2w}}, \qquad \text{if} \quad 0.1 \leqslant w \leqslant w_0.$$

Here w_0 is the unique root of $4w^2 - 188w + 49 = 0$ in the interval $(0,1)$. Moreover, the extremal points are $1,2,3$ if $0 < w < 0.1$, $-2,1,2,3$ if $w = 0.1$, and $-2,1,\xi$ if $0.1 < w \leqslant w_0$. Obviously, $\gamma(w)$ is a differentiable function of w for $0 < w < w_0$, $w \neq 0.1$, but, since

$$\lim_{w \to 0.1-0} \gamma'(w) = 0 \quad \text{and} \quad \lim_{w \to 0.1+0} \gamma'(w) = \tfrac{100}{147},$$

$\gamma(w)$ is not differentiable for $w = 0.1$.

In general, the optimal polynomial for (4.1) can be obtained only numerically. The standard tool for the numerical solution of real linear Chebyshev approximation problems is the method of Remez (see e.g. [12; 20, pp. 105; 27, pp. 163]). For the case $\mu = w = 1$, de Boor and Rice [6] devised a Remez type procedure for the approximation problem (4.1) which exploits the special structure of (4.1). It is straightforward to extend their algorithm to a numerical procedure for the general family (4.1). The reader is referred to [10] for a detailed description of the resulting algorithm. Here, we only outline the basic structure of this numerical approach. Let $\Lambda := (\lambda_0, \lambda_1, \ldots, \lambda_l)$ be any collection of $l+1$ points satisfying (4.3). Using the Lagrange interpolation formula, it is easily verified that for each Λ there exists a unique polynomial $s(\cdot; \Lambda) \in \Pi_{l-1}^{(r)}$ and a unique number $y = y(\Lambda) \in \mathbb{R}$ such that (4.4) holds true. By part (b) of Proposition 4.2, it follows that $s(\cdot; \Lambda^*)$ is the optimal polynomial for (4.1) iff all elements $\lambda_0^*, \ldots, \lambda_l^*$ of Λ^* are extremal points of $f - \lambda s(\lambda; \Lambda^*)$. The algorithm described in [10] is an iterative procedure for computing this optimal Λ^*. By means of a typical Remez exchange step (cf. [20, 27]), in each iteration a collection $\Lambda^{(n)}$ of approximate extremal points is updated. This can be done in such a way that $\Lambda^{(n)}$ converges quadratically to Λ^*.

5. INDEFINITE POLYNOMIAL PRECONDITIONERS

In this section, we return to the polynomial preconditioned MR method for solving the linear system (1.1), $Ax = b$. In particular, the question of how to choose an appropriate polynomial s for the preconditioned system (1.2) or (1.3) is addressed.

As in Section 2, it is always assumed that A is a given indefinite Hermitian $N \times N$ matrix and that $a, b, c, d \in \mathbb{R}$ are known such that

$$\sigma(A) \subset S := [a,b] \cup [c,d], \qquad \text{where} \quad c < d < 0 < a < b \tag{5.1}$$

[cf. (2.4)]. In this paper, we will not consider the problem of how to actually obtain such bounds. The reader is referred to [3, 11], where some results regarding this question can be found.

First, we note that the coefficient matrix $As(A)$ of the preconditioned system (1.2) or (1.3) is Hermitian if, and only if, s is a real polynomial. Therefore, in the following, it is always assumed that $s \in \Pi_{l-1}^{(r)}$, where $l \in \mathbb{N}$ is an arbitrary, but fixed integer. Furthermore, in order to guarantee that $As(A)$ is nonsingular, we require that $s(\lambda) \neq 0$ for all $\lambda \in S$. Since s is continuous and in view of (5.1), this condition implies that there are essentially two different cases: either

$$\lambda s(\lambda) > 0 \qquad \text{for all} \quad \lambda \in S, \tag{5.2}$$

or

$$\lambda s(\lambda) > 0 \quad \text{for all} \ \lambda \in [a,b], \quad \text{and} \quad \lambda s(\lambda) < 0 \quad \text{for all} \ \lambda \in [c,d]. \tag{5.3}$$

Clearly, also the two cases with reversed inequalities may occur, but these can always be reduced to (5.2) respectively (5.3) by replacing s with $-s$.

If (5.2) is satisfied, then, by (5.1), the preconditioned matrix $As(A)$ is positive definite. For the case (5.2), the standard strategy for the choice of the polynomial s is to require that $\lambda s(\lambda)$ approximates the constant function 1 as closely as possible on S. Here, closeness is measured in the uniform norm on S, i.e., s is given as the optimal solution of the approximation problem (4.1), (4.2) with $\mu = w = 1$. This case was studied in detail by Ashby [2] and Ashby, Manteuffel, and Saylor [3].

If (5.3) holds, then, in view of (5.1), the preconditioned system remains indefinite, and we will use the

DEFINITION 5.1. A polynomial $s \in \Pi_{l-1}^{(r)}$ is called an *indefinite polynomial preconditioner* for $Ax = b$ if (5.3) is satisfied.

In the following, we will investigate indefinite polynomial preconditioners and, in particular, develop a strategy for an optimal choice of s.

From now on, it is always assumed that s satisfies (5.3). The criterion for selecting the preconditioner which we will propose here is based only on properties of the coefficient matrix $As(A)$, and hence is the same for left and right polynomial preconditioning (1.2) and (1.3). For simplicity, we will consider only the approach (1.3) in the sequel. More precisely, let $x_0 \in \mathbb{C}^N$ be any initial guess for the solution of $Ax = b$, and let y_n, $n = 1, 2, \ldots$, be the sequence of iterates generated by the MR method [defined via (2.2)] applied to

$$As(A)y = b - Ax_0 \ (=: r_0), \qquad \text{with starting vector} \quad y_0 := 0. \tag{5.4}$$

The iterates and residual vectors corresponding to the original system $Ax = b$ are then given by

$$x_n = x_0 + s(A)y_n \quad \text{and} \quad r_n = b - Ax_n = r_0 - As(A)y_n, \tag{5.5}$$

respectively. Notice that only the iterates y_n are updated at each step. The corresponding approximate solution x_n of $Ax = b$ needs to be computed only once, namely in the very last step of the algorithm. Furthermore, we remark that, in view of (5.5), the residual vectors of y_n [with respect to (5.4)] and of x_n [with respect to $Ax = b$] are identical. This is a slight advantage of right polynomial preconditioning over the approach (1.2).

Next, using the results from Section 2, we state error bounds for the preconditioned MR method. Setting

$$\begin{aligned} \bar{a} &:= \min_{\lambda \in [a,b]} \lambda s(\lambda), \qquad \bar{b} := \max_{\lambda \in [a,b]} \lambda s(\lambda), \\ \bar{c} &:= \min_{\lambda \in [c,d]} \lambda s(\lambda), \qquad \bar{d} := \max_{\lambda \in [c,d]} \lambda s(\lambda), \end{aligned} \tag{5.6}$$

it follows from (5.1) and (5.3) that

$$\sigma(As(A)) \subset \bar{S} := [\bar{a}, \bar{b}] \cup [\bar{c}, \bar{d}] \quad \text{and} \quad \bar{c} < \bar{d} < 0 < \bar{a} < \bar{b}. \tag{5.7}$$

Obviously, the numbers defined in (5.6) depend on s, and we will indicate this, if necessary, by writing $\bar{a}(s), \bar{b}(s), \bar{c}(s), \bar{d}(s)$. Then, in view of (5.7), Theorem 2.1 yields the estimates

$$\frac{\|b - Ax_n\|_2}{\|b - Ax_0\|_2} \leqslant E_n(\bar{a}, \bar{b}, \bar{c}, \bar{d}), \qquad n = 1,2,\ldots. \tag{5.8}$$

Furthermore, by (2.7), the error bound in (5.8) behaves like

$$E_n(\bar{a}, \bar{b}, \bar{c}, \bar{d}) \approx \left[\kappa(\bar{a}, \bar{b}, \bar{c}, \bar{d})\right]^n, \qquad \text{for } n \text{ large.} \tag{5.9}$$

Therefore, (5.8) and (5.9) suggest the following notion of an optimal indefinite polynomial preconditioner.

DEFINITION 5.2. An indefinite polynomial preconditioner $s^* \in \Pi_{l-1}^{(r)}$ is called *optimal* if

$$\kappa(s^*) \leqslant \kappa(s) \tag{5.10}$$

for all indefinite polynomial preconditioners $s \in \Pi_{l-1}^{(r)}$. Here, and in the sequel,

$$\kappa(s) := \kappa(\bar{a}(s), \bar{b}(s), \bar{c}(s), \bar{d}(s)).$$

Finally, we get to the promised connection between indefinite polynomial preconditioners and the family of approximation problems (4.1). Let $(\mu, w) \in \Gamma$, and let $s^*(\lambda) := s_l^*(\lambda; \mu, w)$ be the corresponding optimal polynomial for (4.1). First, we characterize those cases where s^* yields an indefinite preconditioner. With (4.1) and (4.2), it follows that the numbers (5.6) associated with s^* are

$$\bar{a}(s^*) = 1 - \gamma_l(\mu, w), \qquad \bar{b}(s^*) = 1 + \gamma_l(\mu, w),$$

$$\bar{c}(s^*) = \mu - \frac{\gamma_l(\mu, w)}{w}, \qquad \bar{d}(s^*) = \mu + \frac{\gamma_l(\mu, w)}{w}. \tag{5.11}$$

In view of (5.3), (5.6), and (5.11), s^* is an indefinite polynomial preconditioner if, and only if, $(\mu, w) \in \Gamma_l$. Here, we have set

$$\Gamma_l := \{(\mu, w) \in \mathbb{R} \times \mathbb{R} \mid w > 0,\ \gamma_l(\mu, w) < 1, \text{ and } \mu < -\gamma_l(\mu, w)/w\}. \tag{5.12}$$

Moreover, by (5.11), if s^* is an indefinite polynomial preconditioner, then

$$\kappa(s^*) = g_l(\mu, w) := \kappa\left(1 - \gamma_l(\mu, w), 1 + \gamma_l(\mu, w), \mu - \frac{\gamma_l(\mu, w)}{w}, \mu + \frac{\gamma_l(\mu, w)}{w}\right). \tag{5.13}$$

Notice that $g_l(\mu, w)$ is a well-defined function for $(\mu, w) \in \Gamma_l$.

After all these preliminaries, we can now state the main result of this section in the following form.

THEOREM 5.3. *Let* $l \in \mathbb{N}$.

(a) *Let* $s \in \Pi_{l-1}^{(r)}$ *be an indefinite polynomial preconditioner,* $\bar{a}, \bar{b}, \bar{c}, \bar{d}$ *the corresponding numbers defined in* (5.6), *and set*

$$\mu_1 = \frac{\bar{d} + \bar{c}}{\bar{b} + \bar{a}} \quad \text{and} \quad w_1 = \frac{\bar{b} - \bar{a}}{\bar{d} - \bar{c}}. \tag{5.14}$$

Then the optimal polynomial $s^*(\lambda) := s_l^*(\lambda; \mu_1, w_1)$ *of* (4.1) *with parameters* μ_1 *and* w_1 *is an indefinite polynomial preconditioner, and, unless* $s^* \equiv s$,

$$\kappa(s^*) < \kappa(s). \tag{5.15}$$

(b) *There exist parameters* μ_0 *and* w_0 *such that*

$$g_l(\mu_0, w_0) = \min_{(\mu, w) \in \Gamma_l} g_l(\mu, w), \qquad (\mu_0, w_0) \in \Gamma_l. \tag{5.16}$$

(c) *Let* μ_0 *and* w_0 *satisfy* (5.16). *Then the optimal polynomial* $s_l^*(\lambda; \mu_0, w_0)$ *of the approximation problem* (4.1) *with parameters* μ_0 *and* w_0 *is an optimal indefinite polynomial preconditioner.*

Proof. First, we prove part (a). Let $s \in \Pi_{l-1}^{(r)}$ be an indefinite polynomial preconditioner, and hence, by (5.7), $\bar{c} < \bar{d} < 0 < \bar{a} < \bar{b}$. Moreover, by replacing s by $[2/(\bar{a}+\bar{b})]s$, we may assume without loss of generality that

$$\bar{a} + \bar{b} = 2. \tag{5.17}$$

Note that this does not change the asymptotic convergence factor $\kappa(s)$ associated with s. Indeed, it is easily verified that $\kappa(s) = \kappa(\alpha s)$ for all $\alpha \in \mathbb{R} \setminus \{0\}$ and all indefinite polynomial preconditioners s. Now, by using (5.6), (5.14), and (5.17), we obtain

$$\max_{\lambda \in [a,b]} |1 - \lambda s(\lambda)| = \max_{\lambda \in [c,d]} |w_1[\mu_1 - \lambda s(\lambda)]| = \frac{\bar{b} - \bar{a}}{2}. \tag{5.18}$$

In view of (4.1) and (4.2), we conclude from (5.18) that

$$\gamma := \gamma_l(\mu_1, w_1) \leqslant \frac{\bar{b} - \bar{a}}{2} \qquad \text{with " = " holding iff } s \equiv s^*. \tag{5.19}$$

With (5.11), (5.14), and (5.17), it follows from (5.19) that

$$\bar{c}(s) \leqslant \bar{c}(s^*) < \bar{d}(s^*) \leqslant \bar{d}(s) < 0 < \bar{a}(s) \leqslant \bar{a}(s^*) < \bar{b}(s^*) \leqslant \bar{b}(s), \tag{5.20}$$

where, unless $s \equiv s^*$, at least one of the inequalities " $\leqslant$ " is strict. In particular, (5.20) shows that s^* is an indefinite polynomial preconditioner. Moreover, by Proposition 3.4, (5.20) implies (5.15).

We now turn to the proof of part (b). In view of (5.13), (5.12), part (a) of Corollary 3.2, and Lemma 4.4, the function $g_l(\mu, w)$ is continuous on Γ_l. Furthermore, by (2.7), (5.12), and (5.13),

$$g_l(\mu, w) < 1 \qquad \text{for all} \quad (\mu, w) \in \Gamma_l. \tag{5.21}$$

Next, remark that, by (5.12), the boundary $\partial\Gamma_l$ of Γ_l is given by

$$\partial\Gamma_l = \left\{ (\mu, w) \in \mathbb{R} \times \mathbb{R} \;\middle|\; w > 0,\ 1 - \gamma_l(\mu, w) = 0, \text{ and/or } \mu + \frac{\gamma_l(\mu, w)}{w} = 0 \right\}. \tag{5.22}$$

By means of (5.13), (5.22), and part (b) of Corollary 3.2, we conclude that

$$\lim_{(\mu,w)\to(\tilde{\mu},\tilde{w}),\,(\mu,w)\in\Gamma_l} g_l(\mu,w)=1 \qquad \text{for all} \quad (\tilde{\mu},\tilde{w})\in\partial\Gamma_l. \quad (5.23)$$

From (5.21), (5.23), and the continuity of g_l, it follows that g_l attains its minimum on Γ_l, i.e., (5.16) holds true.

Finally, in view of (5.13), (5.10), and (5.15), the statement of part (c) is an immediate consequence of part (a) of this theorem. ■

By means of part (c) of Theorem 5.3, an optimal indefinite polynomial preconditioner can be constructed via the numerical solution of approximation problems of the form (4.1).

6. NUMERICAL EXAMPLES

Based on the connection with the family of approximation problems (4.1), we have computed indefinite polynomial preconditioners in a number of cases. For the solution of (4.1), the Remez procedure described in [10] was used. Optimal indefinite polynomial preconditioners were computed by solving the unconstrained optimization problem (5.16) numerically. Recall (cf. Remark 4.5) that the function g_l in (5.16) is continuous, but only piecewise differentiable. The numerical evaluation of asymptotic convergence factors was done as outlined in Section 3.

In the sequel, we present the results for a typical example. The set S is given by

$$S:=[a,b]\cup[c,d] \qquad \text{with} \quad a=0.01, \quad b=0.99, \quad c=-0.59, \quad d=-0.1. \quad (6.1)$$

The asymptotic convergence factor, which corresponds to no preconditioning, is

$$\kappa(a,b,c,d)=0.9590\ldots.$$

For $l=2,3,\ldots,10$, we have computed indefinite polynomial preconditioners by solving (4.1) with the following parameters. The first choice,

$$\mu_{-1}=-1 \quad \text{and} \quad w_{-1}=1, \quad (6.2)$$

TABLE 1
RESULTS FOR THE THREE STRATEGIES

Polynomial degree	Asymptotic convergence rate		Optimal convergence factor	Parameters in (4.1)	
l	κ_{-1} (6.2)	κ_{-2} (6.3)	κ_{opt}	μ_{opt}	w_{opt}
2	0.986	0.959	0.948	−1.92	0.65
3	0.974	0.936	0.905	−0.68	3.40
4	0.962	0.932	0.874	−2.37	0.74
5	0.957	0.918	0.859	−0.68	5.80
6	0.937	0.908	0.821	−1.92	1.45
7	0.937	0.902	0.820	−1.96	1.40
8	0.922	0.886	0.776	−1.68	2.70
9	0.915	0.885	0.752	−3.78	0.76
10	0.906	0.869	0.734	−1.60	4.40

aims at clustering the positive and negative eigenvalues of $As(A)$ uniformly around 1 and -1, respectively. The resulting asymptotic convergence factor is denoted by κ_{-1} in Table 1. A second obvious strategy is to choose the parameters in (4.1) so that the two intervals (5.7), $\bar{S} := [\bar{a}, \bar{b}] \cup [\bar{c}, \bar{d}]$, containing the eigenvalues of the preconditioned coefficient matrix $As(A)$, have the same relative length and position as the original intervals $[a, b] \cup [c, d]$, i.e.,

$$\frac{b+a}{d+c} = \frac{\bar{b}+\bar{a}}{\bar{d}+\bar{c}} \quad \text{and} \quad \frac{b-a}{d-c} = \frac{\bar{b}-\bar{a}}{\bar{d}-\bar{c}}. \tag{6.3}$$

It is readily verified that (6.3) is fulfilled for the parameters

$$\mu_1 = \frac{d+c}{b+a} \quad \text{and} \quad w_1 = \frac{b-a}{d-c}$$

[cf. part (a) of Theorem 5.3]. The resulting asymptotic convergence factor for this choice will be denoted by κ_1. Note that for the example (6.1) considered here,

$$\mu_1 = -0.69 \quad \text{and} \quad w_1 = 2. \tag{6.4}$$

Finally, via part (c) of Theorem 5.3, we have also computed the optimal asymptotic convergence factor κ_{opt} and the corresponding parameters $\mu_{\text{opt}}, w_{\text{opt}}$ of (4.1). Table 1 lists the results for the three different strategies.

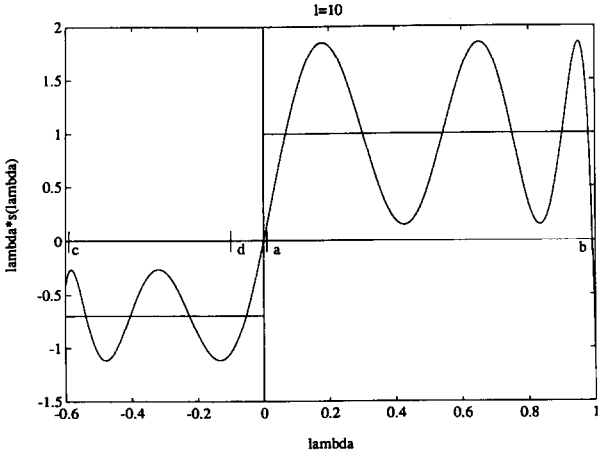

FIG. 1. Plot of the optimal polynomial $\lambda s_{10}^*(\lambda)$ corresponding to $l = 10$ and the strategy (6.3), i.e. $\mu_1 = -0.69$ and $w_1 = 2$.

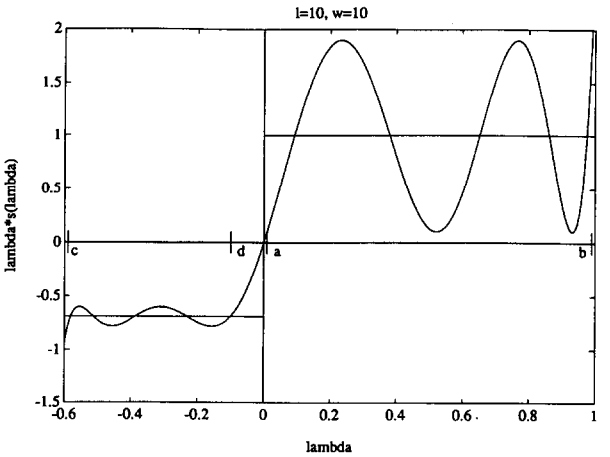

FIG. 2. Plot of the optimal polynomial $\lambda s_{10}^*(\lambda)$ corresponding to $l = 10$ and the parameters $\mu_1 = -0.69$ and $w = 10$.

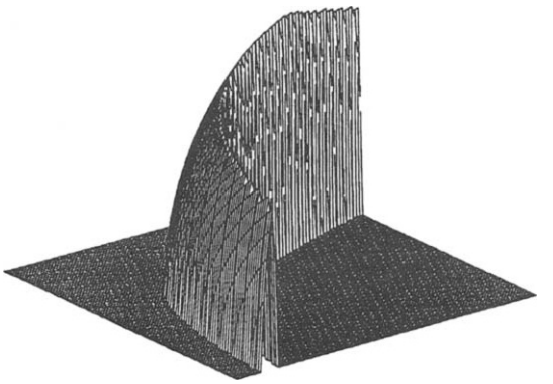

FIG. 3. Plot of the reciprocal asymptotic convergence factor $1/g_l(\mu, w)$ [cf. (5.13)] for $l = 3$.

These results are quite typical for the numerical experiments which we have performed. In particular, they show that the simple strategy (6.2) leads to very poor convergence rates, in particular as l increases. The second strategy leads to better results, but is still by far inferior to the best possible choice. Also notice that the optimal parameters μ_{opt} and w_{opt} exhibit rather erratic behavior as l increases.

The first two plots show, for two cases, the polynomials $\lambda s_{10}^*(\lambda)$ corresponding to the indefinite preconditioned coefficient matrix $As(A)$. Here $s_{10}^*(\lambda)$ denotes the optimal polynomial of (4.1) with $l = 10$. For Figure 1, the

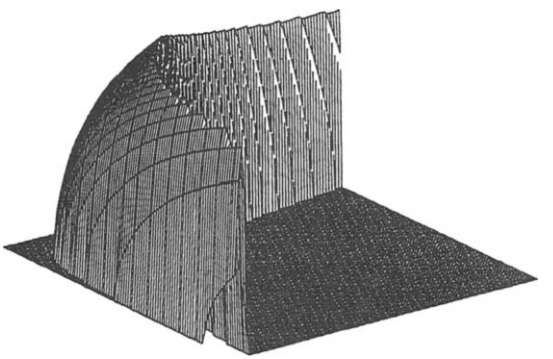

FIG. 4. Plot of the reciprocal asymptotic convergence factor $1/g_l(\mu, w)$ for $l = 10$.

parameters (6.4), $\mu_1 = -0.69$ and $w_1 = 2$, were used. Figure 2 corresponds again to $\mu = \mu_1$, but with increased weight $w = 10$.

Finally, the last two plots show the surface of the function $1/g_l(\mu, w)$ [cf. (5.13)], whose maximum, in view of part (c) of Theorem 5.3, corresponds to an optimal indefinite polynomial preconditioner. For the plots we have set $g_l(\mu, w) = 1$ if $(\mu, w) \notin \Gamma_l$ [cf. (5.12)]. In both cases, the left corner is the point $(\mu, w) = (0, 0)$. The axis pointing towards the reader is the μ-axis. Figure 3 displays the results for $l = 3$, and Figure 4 for $l = 10$.

7. CONCLUDING REMARKS

The standard design of polynomial preconditioners for Hermitian linear systems $Ax = b$ aims at clustering the eigenvalues of the preconditioned matrix around 1. The resulting preconditioned linear system is positive definite then, even if A is indefinite. On the other hand, for indefinite Hermitian A it appears natural to leave the preconditioned system indefinite and to cluster the positive (negative) eigenvalues around 1 (μ), where $\mu < 0$ is some suitable constant. In this paper, we have investigated this second, "indefinite" approach to polynomial preconditioning of Hermitian indefinite linear systems. In particular, it was shown that such indefinite polynomial preconditioners can be constructed via solution of certain Chebyshev approximation problems which depend on two parameters, namely μ and some weighting factor w. This leads to the question of how to select these parameters in order to speed up the iteration optimally. For this task, we have proposed an approach based on the concept of asymptotic convergence factors for two intervals. It was also demonstrated that—based on an explicit representation in terms of elliptic integrals—these asymptotic convergence factors can be very easily computed numerically. Finally, a few numerical examples of indefinite polynomial preconditioners were presented. In a forthcoming paper, we will report on numerical tests for the minimal residual algorithm combined with the indefinite preconditioners developed in this note and compare this approach with other preconditioning strategies for indefinite Hermitian matrices.

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